

MODELLING URBAN AIR POLLUTION

S. HAMEED

Institute for Space Studies, NASA, New York, New York 10025, U.S.A.

(First received 13 April 1973 and in final form 22 November 1973)

Abstract—The performance of simple, one parameter, models for predicting dispersion of air pollutants in urban atmospheres is compared with that of more sophisticated methods. It is concluded that presently available simple models are not dependable enough to preclude the development of more complex models.

1. INTRODUCTION

In recent years a number of models have been developed to predict the dispersion of contaminants in urban atmospheres. These models range in complexity from those designed to solve the three-dimensional diffusion equation to models containing only one parameter. In this paper we compare the performance of some theoretical models of varying complexity and draw conclusions about their suitability. These calculations predict the dispersion of SO_2 during a period of 2 h (16:00 – 18:00 CST) on 11 January 1959 in the atmosphere of Nashville, Tennessee, a city for which more than usual amount of relevant data are available.

2. COMPARISON

Randerson (1968, 1970) approached this problem by numerically solving the three dimensional diffusion equation, including the effects of horizontal and vertical advection and chemical decay, thus predicting the evolution of the concentration pattern of SO_2 for the 2-h period. Halliday and Ventner (1971) have criticised this calculation by suggesting that concentration values, X , obtained by the simple formula

$$X = Q/u \quad (1)$$

where Q is the local source strength and u the mean wind speed, are as good as those of the detailed model of Randerson. Gifford and Hanna (1973) have invoked the argument of Halliday and Ventner in support of their own model according to which,

$$X = cQ/u, \quad (2)$$

where the constant of proportionality c is

$$c = (2/\pi)^{1/2} x^{(1-b)} [a(1-b)]^{-1}, \quad (3)$$

where x is the distance from a receptor point to the upwind edge of the area source. Models similar to equation (2) have been used for many years. (See, for instance, Smith, 1961 and Miller and Holzworth, 1967). The constants a and b are defined by the vertical atmospheric diffusion length, $\sigma = ax^b$. In another paper Gifford and Hanna (1971) have suggested that

the atmosphere over an urban area belongs to the meteorological class called "slightly stable" for which the values of the constants are

$$a = 0.15; \quad b = 0.75.$$

Gifford and Hanna (1973) suggest that their simple model, given by equations (2 and 3), predicts pollutant concentrations at least as well as more detailed calculations, and that their model is valid for calculation of both long term (such as annual) pollution concentrations and short term (such as over a few hours) concentrations. From these considerations they conclude that efforts to develop more sophisticated models for simulating pollution dispersion are not necessary. In the comparison which follows it appears that the claims in favor of the simple models are not quite justified.

Concerning the criticism of Halliday and Ventner (1971) it may be noted that, when comparing their formula, $X = Q/u$, with the results of Randerson they have not used consistent units. While concentrations given by Randerson are in pphm, Halliday and Ventner have taken Q in $\text{g SO}_2 \text{ s}^{-1} \text{ mile}^{-2}$ and the velocity u in m s^{-1} . By converting Q to $\text{g s}^{-1} \text{ m}^{-2}$ and taking the density of air to be 1230 g m^{-3} , and the molecular weights of SO_2 and air to be 64 and 29 respectively, we have expressed Halliday and Ventner's results in pphm and these are compared with those of Randerson's in Table 1. On using consistent units, and a wind speed of 2 m s^{-1} , it is obvious that Randerson's results are in much better agreement with observations.

In column (6) of Table 1 we list the concentrations according to equations (2 and 3). It is seen that the model of Gifford and Hanna greatly overestimates the values for the concentration. In any case, the results obtained by Randerson are in much better agreement with observations as compared to the results of the simple models of equations (1 and 2). It may be noted that chemical decay of SO_2 was calculated by Randerson. It resulted in an overall loss of 12 per cent of SO_2 , the values at individual observation stations being reduced by between 10 and 20 per cent. For the prevailing values of SO_2 concentration, in this episode of 2 h, Randerson's estimate of the effects of chemical decay appears to be plausible. Inclusion of this effect in the results of column (6) would still leave the predictions of equation (2) far in excess of observed values. It may be noted here that the models given by equations (1 and 2) are designed for sources of uniform area type only. The effects of point sources, if any, have to be added separately. The plume from a point source gives higher concentrations in a narrower pencil downwind of the source as compared to an area source, of the same strength, which results in weaker concentrations spread over a larger volume downwind of the source. The emission inventory for Nashville (Stalker *et al.*, 1964) used in the calculations discussed in this paper does not contain point sources.

It should be mentioned here that Randerson's calculation was one of the early attempts at numerically solving the diffusion equation for estimating urban pollution dispersion. It suffers from several drawbacks, the principal one being the confinement of the vertical spread of the model to 60 m above the base of the model. This vertical confinement leads to a restriction in the movement of SO_2 in the model and therefore distorts the concentration distribution. This, however, points to an important difference between comprehensive and simple models. A model in which an effort is made to systematically consider the various physical and chemical processes which are responsible for dispersion is helpful in the understanding of the rôles played by these processes and thus allows us to analyze the reasons for the shortcomings of the model and the methods by which they may be corrected.

Table 1. Comparison of observed concentrations of SO_2 in Nashville with predictions of several theoretical models. Concentrations are expressed in pphm. (1 pphm is equivalent to $2.7 \times 10^{-5} \text{ g m}^{-3}$ of SO_2)

Observation station	Initial concentration (observed)	Observed final concentration	Numerical model of Randerson	$X = Q/u$ equation (1)	Gifford and Hanna model equations (2 and 3)	Multi-cell model	Persistence
19	3.5	5.8	5.1	0.22	45	4.0	3.5
48	5.8	13.6	6.5	0.23	50	7.3	5.8
52	0.0	2.9	0.4	0.19	28	3.2	0.0
56	2.0	6.9	0.9	0.015	3.6	5.9	2.0
60	14	20.9	14.0	0.40	84	6.8	14
82	5.5	13.2	4.2	0.35	69	3.6	5.5
90	3.5	4.1	2.7	0.15	32	2.9	3.5
	Correlation coefficient		0.89	0.74	0.81	0.70	0.93
	Mean relative error		-0.53	-0.97	4.5	-0.33	-0.56

For further comparison we present also in Table 1 the results obtained for the same problem by the use of a multi-cell model. (Hameed, 1974). In this method the area under study is divided into control volumes, or cells, of 1 mile² each. In each of these cells pollutant concentration is assumed to be horizontally uniform and to have a Gaussian distribution in the vertical direction. This calculation neglects the effects of horizontal turbulent diffusion and those of chemical decay. It is intermediate in complexity between the comprehensive and very simple models discussed above.

3. INDICES FOR GOODNESS OF PREDICTION

In the bottom two rows of Table 1 we present, for each calculation, the correlation coefficient and the mean relative error. It may be noted that the correlation coefficient, being independent of an arbitrary multiplicative factor in either of the sets of numbers being studied, is not, by itself, a sufficiently transparent index for indicating the success of a prediction. It is important to consider also a measure of relative magnitudes, such as the mean relative error. For instance, although the correlation coefficients of Randerson's numerical model and Gifford and Hanna's model are comparable, their relative mean errors are very different, being -0.53 and 4.5 respectively. They show that, on the average, values predicted by Randerson's calculation are nearly $1/2$ those of the observed ones, while the predictions of Gifford and Hanna model are, on the average, 5.5 times the observations.

An objective method of judging the predictive skill of a model is to test its performance against a persistence forecast, which in the present case is given in column (8) of Table 1. If the proposed model cannot forecast the specified parameters better than persistence then the model is of questionable value. Table 1 shows that in terms of the correlation coefficient, persistence outperforms all the models considered, while in terms of the relative error, the multi-cell model appears to be the best. In fact the relevance of the initial values of concentration with respect to the simple models is not clear. Under steady-state conditions persistence is likely to be a good forecast. One could make a *post facto* calculation of the constant c in equation (2) based on the known initial conditions. Such a procedure would yield impressive values of the correlation coefficient and the mean relative error, but these values would only be as good as a persistence forecast, not better.

4. FURTHER SIMPLIFICATION

Gifford and Hanna (1973) have introduced a further simplification of their model. They have tabulated, the total annual pollutant emissions, annual average wind velocities, the annual average pollutant concentrations and the areas for many cities in the United States. Assuming that these data should conform to their model, i.e. equation (2), they have computed the constant c for each of the cities from the tabulated values of X , Q and u . They then have averaged over these values of c and proposed that equation (2), with the resulting value of c , gives a general model for predicting urban air pollution. They have carried out this procedure for two types of pollutants, oxides of sulfur (SO_x) and particulate matter.

Oxides of sulfur

For SO_x the resulting equation obtained from data for 20 cities is:

$$X = 50 Q/u \mu\text{g m}^{-3}. \quad (4)$$

The correlation coefficient between X and Q/u for these 20 cities is 0.15 . Now, if two variables are totally uncorrelated, the probability that a random sample of 20 observations

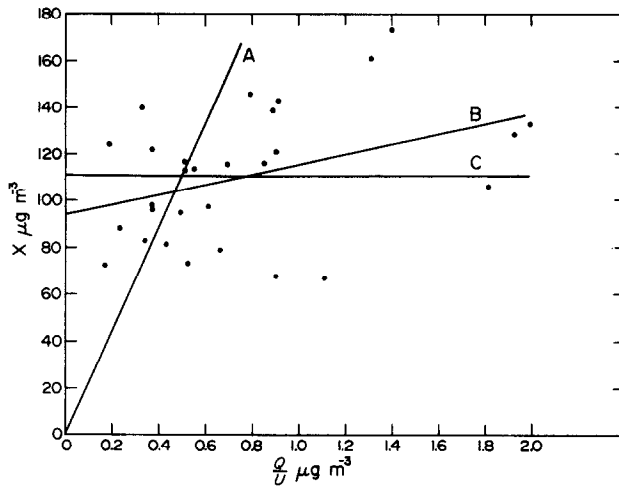


Fig. 1. Observed annual average particulate concentration (X) is plotted against Q/u for 29 U.S. cities. The lines show three linear relationships between these quantities, (A) $X = 225 Q/u$, equation (5), (B) $X = 94 + 22 Q/u$ (least squares fit), equation (6), (C) $X = 111$ (average X), equation (7).

will yield a correlation coefficient greater than 0.15 is greater than 50 per cent (Bevington, 1969). It is obvious therefore that a linear relation between X and Q/u is not supported by the SO_x data.

Particulate matter

For particulate matter the equation with the average c , obtained from data for 29 cities, is

$$X = 225 Q/u \mu\text{g m}^{-3}. \quad (5)$$

The correlation coefficient between X and Q/u in this case is 0.40 which means that a linear relationship though weak, is not negated by the data. An objective look at the data shows, however, that the deduction of equation (5) from these data is not justified. This is seen in Fig. 1 where the points show the observed X plotted against the observed Q/u and line (A) represents equation (5).

If one wishes to assume a linear relationship between X and Q/u then the "best" such line would be obtained by a least squares fit, which gives

$$X = 94 + 22 Q/u \mu\text{g m}^{-3}. \quad (6)$$

This line is shown as (B) in Fig. 1. The small value of the slope indicates that assuming X to be simply a constant is, objectively, a better representation of the data than equation (5). The average of the observed concentrations, X , is $111 \mu\text{g m}^{-3}$, and the horizontal line (C), which represents

$$X = 111 \mu\text{g m}^{-3} \quad (7)$$

is also shown in Fig. 1. The predictive capabilities of the three formulae, equations (5, 6 and 7) are compared in Table 2 where the mean relative error and the standard error of estimate are given for the three formulae. It is apparent that the statistics do not support equation (5).

Table 2. Comparison of three formulas, equations (5, 6 and 7), for predicting annual average particulate concentration in 29 U.S. cities

Formula	Index	
	Mean relative error	Standard error of estimate
$X = 225 Q/u$, equation (5)	0.56	124
$X = 94 + 22 Q/u$, equation (6) (least squares fit)	0.06	26
$X = 111$, equation (7) (average value)	0.07	29

5. CONCLUSIONS

Generally speaking, the case of Nashville discussed above illustrates that, at least in some cases, urban air pollution modelling is a complex forecasting problem and simple considerations like those of equations (1 and 2) are not sufficient to cope with it. As Gifford and Hanna point out, most current detailed models of urban air pollution predict concentrations with errors, on the average, of the order of a factor of 2. This is because of the poor quality of data and also because dispersion modelling is still a developing technique. Most of currently available data are such that a prediction better than with an error of a factor of 2 may be regarded as fortuitous. This does not mean, however, that there is no need for developing models which take account of the complexities of meteorological, topographical or of other types, which determine the dispersion of pollutants. If dispersion modelling is to play a useful rôle in urban planning or in devising pollution control strategies, it is necessary that *reliable* models of atmospheric dispersion be available. While a sophisticated model developed for a particular situation can be depended upon to predict pollution concentration to within a factor of, say, 2 on the average, it is apparent from considerations discussed above that simple models like equations (1 and 2) or (5) cannot be relied upon to give results which are *always* correct to within a given margin of error. Accuracy of detailed dispersion models is likely to increase as more and better data become available. Moreover, a comprehensive dispersion model for a given location need to be constructed only once, after which it can be used continuously with updated source information and a predicted flow field to monitor and simulate the expected pollution field. It is of course possible that under certain conditions simple models may give results comparable to more sophisticated methods, but until such conditions are clearly understood and categorized one cannot depend upon the simple models.

Acknowledgements—The author wishes to thank Dr. D. Randerson of the Air Resources Laboratory of the U.S. Department of Commerce for very useful discussions about this work.

REFERENCES

- Bevington P. R. (1969) *Data Reduction and Error Analysis for the Physical Sciences*, pp. 310–312. McGraw-Hill, New York.
- Gifford F. A. and Hanna S. R. (1971) Urban air pollution modelling. *Proceedings of The 2nd International Clean Air Congress* (Edited by Englund H. M. and Beery W. T.), pp. 1146–1151.
- Gifford F. A. and Hanna S. R. (1973) Modelling urban air pollution. *Atmospheric Environment* 7, 131–136.
- Halliday E. C. and Ventner G. (1971) A numerical experiment in simulating the transport of sulfur dioxide through the atmosphere. *Atmospheric Environment* 5, 815–818.
- Hameed S. (1974) A multi-cell method for simulation of atmospheric transport. *Atmospheric Environment*, to be published.

- Miller M. E. and Holzworth G. C. (1967) An atmospheric diffusion model for metropolitan areas. *J. Air Pollut. Control Ass.* **17**, 46–50.
- Randerson D. (1968) A numerical model for predicting the transport of sulfur dioxide through the atmosphere. Ph.D. dissertation, Texas A & M University, 153 pp.
- Randerson D. (1970) A numerical experiment in simulating the transport of sulfur dioxide through the atmosphere. *Atmospheric Environment* **4**, 615–632.
- Smith M. (1961) The concentrations and residence times of pollutants in the atmosphere. *Chemical Reactions in the Lower and Upper Atmosphere*, pp. 155–166. Interscience, New York.
- Stalker W. W., Kenline P. A. and Paulus H. J. (1964) Nashville sulfur dioxide emission inventory and the relationship to measured sulfur dioxide. *J. Air Pollut. Control Ass.* **14**, 469–474.